

# Monte Carlo Hamiltonian: Generalization to Quantum Field Theory

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Monte Carlo techniques with importance sampling have been extensively applied to lattice gauge theory in the Lagrangian formulation. Unfortunately, it is extremely difficult to compute the excited states using the conventional Monte Carlo algorithm. Our recently developed approach: the Monte Carlo Hamiltonian method, has been designed to overcome the difficulties of the conventional approach. In this paper, we extend the method to many body systems and quantum field theory. The Klein-Gordon field theory is used as a testing ground.

## 1 Introduction

Quantum theory is one of the most important achievements in modern science, but a lot of non-perturbative aspects are still poorly understood. There are two standard formulations in quantum theory: Hamiltonian and Lagrangian. A comparison of the conventional approaches is given in Tab.1.

The Lagrangian formulation is very suitable for applying the Monte Carlo (MC) method to systems with many degrees of freedom, and in the last two decades, it has been widely applied to lattice gauge theory<sup>1,2,3</sup>. In the standard Lagrangian MC method, however, it is extremely difficult to compute the spectrum and wave function beyond the ground state. On the other hand, the standard Hamiltonian formulation is capable of doing it. In fact, some efforts have been made to solve the lattice QCD Schrödinger equation<sup>4</sup>. But due to the complexity of non-Abelian gauge theory and high degrees of freedom, only the ground state<sup>5</sup> and the lowest lying glueball states<sup>6,7,8</sup> have been investigated. There have also been some attempts to perform numerical simulations in the Hamiltonian formulation, e.g. the quantum MC technique<sup>9</sup>, MC method using a guided random walk<sup>10,11</sup>, and the MC Green's function method<sup>12,13</sup>. For an review of MC methods applied to solve the quantum many-body problem see Ref.<sup>14</sup>.

Table 1. Comparison of the conventional methods in the standard formulations.

Formulation	Hamiltonian	Lagrangian
Approach	Schrödinger Eq. $H E_n\rangle = E_n E_n\rangle$	Path Integral $\langle O \rangle = \frac{\int [d\varphi] O[\varphi] \exp(-S[\varphi]/\hbar)}{\int [d\varphi] \exp(-S[\varphi]/\hbar)}$
Algorithm	Series expansion, variational, Runge-Kutta ...	MC simulation
Advantage	Both the ground state, and the excited states can be computed.	It generates the most important configs. for the measurements.
Disadvantage	Analytical methods are too tedious for many body systems; Runge-Kutta works only in 1-D.	It is difficult to study the excited states, and finite density QCD.

A natural question is whether in Lagrangian MC simulations one can construct an effective Hamiltonian? If yes, the excited states can also be computed. We have recently proposed a new approach<sup>15</sup> (we called it Monte Carlo Hamiltonian method) to investigate this problem. A lot of models<sup>15,16,17,18,19,20</sup> in quantum mechanics (QM) have been used to test the method, as briefly reviewed in Sect. 2. In this paper, we will extend the method to many body systems and quantum field theory (QFT).

## 2 Algorithm

### 2.1 Effective Hamiltonian

The basic idea of the MC Hamiltonian method for one body quantum mechanics has been described in details in Ref.<sup>15</sup>. The (imaginary time) transition amplitude between an initial state at position  $x_i$ , and time  $t_i$ , and final state at  $x_f$  and  $t_f$  is related to the Hamiltonian  $H$  by

$$\begin{aligned}
 M_{fi} &= \langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-H(t_f - t_i)/\hbar} | x_i \rangle \\
 &= \sum_{n=1}^{\infty} \langle x_f | E_n \rangle e^{-E_n T/\hbar} \langle E_n | x_i \rangle,
 \end{aligned} \tag{1}$$

where  $T = t_f - t_i$ . According to Feynman's path integral formulation of QM, the transition amplitude is also related to the path integral:

$$M_{fi} = \int [dx] \exp(-S[x]/\hbar) |_{x_i, t_i}^{x_f, t_f}, \quad (2)$$

where  $S = S_0 + S_V$  is the action for a given path,  $S_0 = \int_{t_i}^{t_f} dt \, m\dot{x}^2/2$ , and  $S_V = \int_{t_i}^{t_f} dt \, V(x)$ .

The results above are standard ones in Lagrangian formulations. What is new in our method<sup>15</sup> is to construct an effective Hamiltonian  $H_{\text{eff}}$  (finite  $N \times N$  matrix) through

$$M_{fi} = \langle x_f | e^{-H_{\text{eff}}T/\hbar} | x_i \rangle = \sum_{n=1}^N \langle x_f | E_n^{\text{eff}} \rangle e^{-E_n^{\text{eff}}T/\hbar} \langle E_n^{\text{eff}} | x_i \rangle. \quad (3)$$

The eigenvalues  $E_n^{\text{eff}}$  and wave function  $|E_n^{\text{eff}}\rangle$  can be obtained, by diagonalizing  $M$  using a unitary transformation  $M = U^\dagger D U$ , where  $D = \text{diag}(e^{-E_1^{\text{eff}}T/\hbar}, \dots, e^{-E_N^{\text{eff}}T/\hbar})$ . Once the spectrum and wave functions are available, all physical information can also be obtained.

Since the theory described by  $H$ , which has an infinite basis in Hilbert space, is now approximated by a theory described by a finite matrix  $H_{\text{eff}}$ , which has a finite basis, the physics of  $H$  and  $H_{\text{eff}}$  might be quite different at high energy. Therefore we expect that we can only reproduce the low energy physics of the system. This is good enough for our purpose. In Refs.<sup>15,16,17,18,19,20</sup>, we investigated many 1-D, 2-D and 3-D QM models (Tab.2) using this MC Hamiltonian algorithm. We computed the spectrum, wave functions and some thermodynamical observables. The results are in very good agreement with those from analytical and/or Runge-Kutta methods.

## 2.2 Basis in Hilbert Space

To get the correct scale for the spectrum, the position state  $|x_n\rangle$  at initial time  $t_i$  or final time  $t_f$  (Bargman states or box states) should be properly normalized. We denote a normalized basis of Hilbert states as  $|e_n\rangle$ ,  $n = 1, \dots, N$ . In position space, it can be expressed as

$$e_n(x) = \begin{cases} 1/\sqrt{\Delta x_n}, & x \in [x_n, x_{n+1}] \\ 0, & x \notin [x_n, x_{n+1}] \end{cases} \quad (4)$$

where  $\Delta x_n = x_{n+1} - x_n$ .

There is some arbitrariness in choosing a basis for the initial and final states. The simplest choice is a basis with  $\Delta x_n = \text{const.}$ , which is called the

Table 2. QM systems, investigated by the MC Hamiltonian method with a regular basis.

System	Potential
QM in 1-D	$V(x) = 0$ $V(x) = \frac{1}{2}m\omega^2x^2$ $V(x) = -V_0\text{sech}^2(x)$ $V(x) = \frac{1}{2}x^2 + \frac{1}{4}x^4$ $V(x) = \frac{1}{2} x $ $V(x) = \begin{cases} \infty, & x < 0 \\ Fx, & x \geq 0 \end{cases}$
QM in 2-D	$V(x, y) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2$ $V(x, y) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2 + \lambda xy$
QM in 3-D	$V(x, y, z) = \frac{1}{2}m\omega^2x^2 + \frac{1}{2}m\omega^2y^2 + \frac{1}{2}m\omega^2z^2$

“regular basis”. In Refs.<sup>15,16,17,18</sup>, the regular basis was used. For many body systems or QFT, the regular basis will encounter problems. For example, in a system with a 1-D chain of oscillators (see later), if the number of oscillators is 30, the minimum non-trivial regular basis is  $N = 2^{30} = 1073741824 \approx 10^9$ , which is prohibitively large for numerical calculations of the matrix elements.

Guided by the idea of importance sampling, in Refs.<sup>19,20</sup>, we proposed to select a basis from the Boltzmann weight proportional to the transition amplitude between  $x'_i = 0$  at  $t'_i = 0$  and  $x'_f = x_n$  at some  $t'_f$ . In a free particle or harmonic oscillator case, the distribution is just a Gaussian

$$P_{basis}[x_n] = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x_n^2}{2\sigma^2}\right), \quad (5)$$

where  $\sigma = \sqrt{\hbar T'/m}$  for the free case and  $\sigma = \sqrt{\hbar \sinh(\omega T')/(m\omega)}$  for the harmonic oscillator. We call such a basis the “stochastic basis”, to be used as states at initial time  $t_i$  or final time  $t_f$ . For more complicated models, one may still use the Gaussian distribution, but with an adjustable parameter  $\sigma$ .

### 2.3 Matrix elements

As explained above, the calculation of the transition matrix elements is an essential ingredient of our method. The matrix element in the normalized basis is related to  $\langle x_{n'}, t_f | x_n, t_i \rangle$  by

$$M_{n'n} = \langle e_{n'}, t_f | e_n, t_i \rangle = \int_{x'_n}^{x_{n'+1}} dx' \int_{x_n}^{x_{n+1}} dx'' \frac{\langle x', t_f | x'', t_i \rangle}{\sqrt{\Delta x_{n'} \Delta x_n}}$$

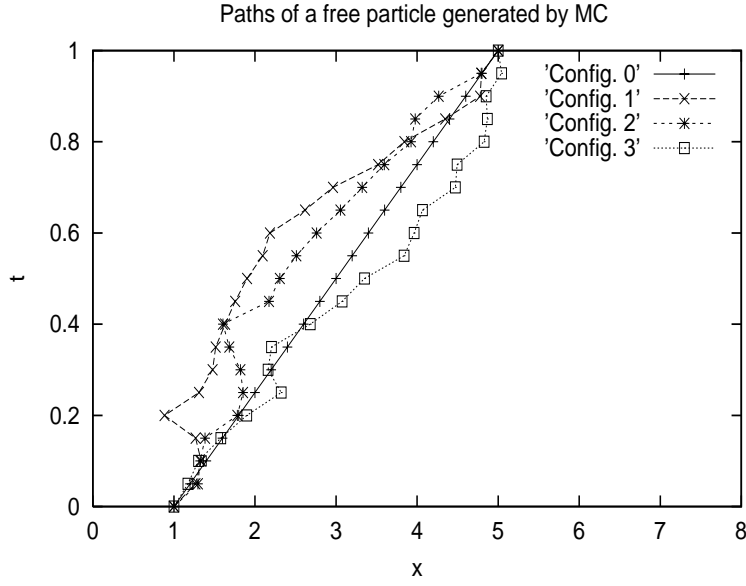


Figure 1. Config. 0 stands for the classical path, Config. 1, Config. 2 and Config. 3 stand the paths generated by MC. Here  $N_t = 20$  (there are 19 time slices between  $t_i$  and  $t_f$ ).

$$\approx \sqrt{\Delta x_{n'} \Delta x_n} \langle x_{n'}, t_f | x_n, t_i \rangle, \quad (6)$$

where for the regular basis,  $\Delta x_n = \text{const.}$ , and for a stochastic basis,  $\Delta x_n = 1/(P_{basis}[x_n]N)$ .  $\langle x_{n'}, t_f | x_n, t_i \rangle$  can be calculated by MC as follows.

- (a) Discretize the continuous time with time interval  $\Delta t = T/N_t$ .
- (b) Generate free configurations  $[x]$  between  $t \in (t_i, t_f)$  obeying the Boltzmann distribution

$$P_0[x] = \frac{\exp(-S_0[x]/\hbar)}{\int [dx] \exp(-S_0[x]/\hbar)} \Big|_{x_n, t_i}^{x_{n'}, t_f}. \quad (7)$$

Figure 1 shows a sample of free configurations generated by MC method with importance sampling.

- (c) Measure

$$\langle O_V \rangle = \int [dx] \exp(-S_V(x)/\hbar) \Big|_{x_n, t_i}^{x_{n'}, t_f} P_0[x]. \quad (8)$$

The path integral in Eq. (6) is then

$$\langle x_{n'}, t_f | x_n, t_i \rangle = \langle O_V \rangle \sqrt{\frac{m}{2\pi\hbar T}} \exp \left[ -\frac{m}{2\hbar T} (x_{n'} - x_n)^2 \right]. \quad (9)$$

### 3 Quantum Field Theory

#### 3.1 The Klein-Gordon model

The main purpose of the algorithm is to study many body systems and QFT. As an example, we consider a free scalar field theory: the Klein-Gordon model in 1+1 dimensions, which has the Hamiltonian

$$H = \int dx \frac{1}{2} \left( \pi^2 + \nu^2 \left( \frac{\partial \varphi}{\partial x} \right)^2 + \Omega_0^2 \varphi^2 \right). \quad (10)$$

Discretizing the theory on a finite string with  $N_{\text{osc}}$  sites and lattice spacing  $a$ , and making the replacement  $x \rightarrow x_j = ja$ ,  $\pi(x) \rightarrow a^{-1/2} \Pi(x_j)$ ,  $\varphi(x) \rightarrow a^{-1/2} \phi(x_j)$ ,  $\int \rightarrow a \sum_{j=1}^{N_{\text{osc}}}$  and  $\nu \rightarrow a\Omega$ , the Hamiltonian becomes

$$H = \sum_{j=1}^{N_{\text{osc}}} \frac{1}{2} \left( \Pi^2(x_j) + \Omega^2 (\phi(x_j) - \phi(x_{j+1}))^2 + \Omega_0^2 \phi^2(x_j) \right), \quad (11)$$

which describes a chain of  $N_{\text{osc}}$  coupled oscillators<sup>21</sup> with  $m = 1$  in 1 spatial dimension. The field  $\phi(x_j)$  and its conjugate momentum  $\Pi(x_j) = \dot{\phi}(x_j)$  at the  $j$ -th site correspond respectively to the displacement and velocity of the  $j$ -th oscillator.

In QFT, the initial and final states are defined by

$$\begin{aligned} |\Phi_i, t_i\rangle &= |\phi(x_1, t_i), \dots, \phi(x_{N_{\text{osc}}}, t_i)\rangle, \\ |\Phi_f, t_f\rangle &= |\phi(x_1, t_f), \dots, \phi(x_{N_{\text{osc}}}, t_f)\rangle. \end{aligned} \quad (12)$$

The transition amplitude between them is

$$\begin{aligned} M_{fi} &= \langle \Phi_f, t_f | \Phi_i, t_i \rangle = \langle \Phi_f | e^{-H(t_f - t_i)/\hbar} | \Phi_i \rangle \\ &= \int [d\phi] \exp(-S[\phi]/\hbar) |_{\phi_i, t_i}^{\phi_f, t_f} \\ &= \lim_{N_t \rightarrow \infty} \int \prod_{k=1}^{N_t-1} \prod_{j=1}^{N_{\text{osc}}} \left( \sqrt{\frac{1}{2\pi\hbar\Delta t}} d\phi(x_j, t_k) \right) \exp(-S[\phi]/\hbar), \end{aligned} \quad (13)$$

where the Euclidean action is

$$S = \frac{\Delta t}{2} \sum_{k=1}^{N_t-1} \sum_{j=1}^{N_{\text{osc}}} \left[ \frac{(\phi(x_j, t_{k+1}) - \phi(x_j, t_k))^2}{(\Delta t)^2} + \Omega^2 (\phi(x_j, t_k) - \phi(x_{j+1}, t_k))^2 + \Omega_0^2 \phi^2(x_j, t_k) \right]. \quad (14)$$

For a finite  $N_{\text{osc}}$  and non-zero  $\Omega$ , one has to introduce a boundary condition for  $\phi(x_{N_{\text{osc}}+1})$ . We implement the periodic boundary condition  $\phi(x_{N_{\text{osc}}+1}) = \phi(x_1)$ . The spectrum is analytically known<sup>21</sup>:

$$E_n = \sum_{n_l} \left( n_l + \frac{1}{2} \right) \hbar \omega_l, \quad (15)$$

where  $\omega_l = \sqrt{\Omega_0^2 + 4\Omega^2 \sin^2(p_l \Delta x / 2)}$ , and  $n_1, \dots, n_{N_{\text{osc}}} = 0, 1, \dots$ . We can also compute the transition amplitude analytically, using the discrete Fourier transformation

$$\begin{aligned} \phi(x_j, t) &= \sum_l \frac{\Delta p}{\sqrt{2\pi}} \exp(ip_l x_j) \tilde{\phi}(p_l, t), \\ \tilde{\phi}(p_l, t) &= \sum_j \frac{\Delta x}{\sqrt{2\pi}} \exp(-ip_l x_j) \phi(x_j, t), \end{aligned} \quad (16)$$

where  $\Delta x = a$ ,  $\Delta p = 2\pi/(N_{\text{osc}} \Delta x)$ ,  $x_j = [-(N_{\text{osc}} - 1)/2 + (j - 1)]\Delta x$ ,  $p_l = [-(N_{\text{osc}} - 1)/2 + (l - 1)]\Delta p$ , and  $j, l = 1, \dots, N_{\text{osc}}$ . The result is

$$\begin{aligned} M_{fi} &= \prod_{l=1}^{N_{\text{osc}}} \sqrt{\frac{m\omega_l}{2\pi\hbar \sinh(\omega_l T)}} \exp \left[ -\frac{\omega_l \Delta p / \Delta x}{2\hbar \sinh(\omega_l T)} \right. \\ &\quad \times \left. \left( |\tilde{\phi}(p_l, t_f)|^2 + |\tilde{\phi}(p_l, t_i)|^2 \right) \cosh(\omega_l T) - 2\text{Re} \left( \tilde{\phi}(p_l, t_f) \tilde{\phi}^*(p_l, t_i) \right) \right]. \end{aligned} \quad (17)$$

### 3.2 Stochastic basis

In QFT, a stochastic basis has to be used for the initial and final states, because in the thermodynamical limit,  $N_{\text{osc}} \rightarrow \infty$ . Although the variables  $\phi$  are coupled in position space, we may still use a stochastic basis  $[\Phi_n]$ ,  $n = 1, \dots, N$  according to the distribution with an adjustable parameter  $\sigma$

$$P_{\text{basis}}[\Phi_n] = \prod_{j=1}^{N_{\text{osc}}} \frac{1}{\sqrt{2\pi\sigma}} \exp \left( -\frac{\phi_n^2(x_j)}{2\sigma^2} \right). \quad (18)$$

The matrix element between the normalized initial and final states is

$$M_{n'n} = \langle e_{n'}, t_f | e_n, t_i \rangle \approx \sqrt{\Delta\Phi_{n'} \Delta\Phi_n} \langle \Phi_{n'}, t_f | \Phi_n, t_i \rangle, \quad (19)$$

where the infinitesimal volumes for the initial and final states are

$$\begin{aligned} \Delta\Phi_n &= d\phi_n(x_1) \dots d\phi_n(x_{N_{\text{osc}}}) = \frac{1}{P_{\text{basis}}[\Phi_n]N}, \\ \Delta\Phi_{n'} &= d\phi_{n'}(x_1) \dots d\phi_{n'}(x_{N_{\text{osc}}}) = \frac{1}{P_{\text{basis}}[\Phi_{n'}]N}. \end{aligned} \quad (20)$$

## 4 Results

We consider  $N_{\text{osc}} = 9$ ,  $a = 1$ ,  $\Omega = 1$ ,  $\Omega_0 = 2$ ,  $m = 1$ ,  $\hbar = 1$ , and  $T = 2$ . For the adjustable parameter  $\sigma$  in the stochastic basis, we choose  $\sigma = \sqrt{\hbar \sinh(\Omega_0 T') / (m \Omega_0)}$  with  $T' = T$  for simplicity. After the stochastic basis with  $N = 1000$  is generated, we obtain the matrix elements  $M_{n'n}$  using Eqs. (17), (19) and (20). (In the future work, we will calculate  $\langle \Phi_{n'}, t_f | \Phi_n, t_i \rangle$  directly by MC). Then we compute the eigenvalues and eigenvectors using the method described in Sect. 2.1.

Table 3 gives a comparison between the spectrum from the effective Hamiltonian with the stochastic basis and the analytical formular Eq. (15) for the first 20 states. They agree very well. This means that an arbitrary choice of Gaussian distribution for the stochastic basis is good enough. (Of course, one should study systematically the dependence of the results on  $\sigma$ ).

We have also computed thermodynamical quantities such as the partition function  $Z$ , average energy  $\bar{E}$  and specific heat  $C$ . The analytical results are

$$\begin{aligned} Z(\beta) &= \text{Tr}(\exp(-\beta H)) = \prod_{l=1}^{N_{\text{osc}}} \frac{1}{2 \sinh(\beta \hbar \omega_l / 2)}, \\ \bar{E}(\beta) &= \frac{1}{Z} \text{Tr}(H \exp(-\beta H)) = -\frac{\partial \log Z}{\partial \beta} = \sum_{l=1}^{N_{\text{osc}}} \frac{\hbar \omega_l}{2} \coth(\beta \hbar \omega_l / 2), \\ C(\beta) &= k_B \frac{\partial \bar{E}}{\partial T} = -k_B \beta^2 \frac{\partial \bar{E}}{\partial \beta} = k_B \sum_{l=1}^{N_{\text{osc}}} \left( \frac{\beta \hbar \omega_l / 2}{2 \sinh(\beta \hbar \omega_l / 2)} \right)^2, \end{aligned} \quad (21)$$

where  $\beta = T/\hbar$ , the temperature  $T = 1/(\beta k_B)$ , and  $k_B$  is the Boltzmann constant. Since we have approximated  $H$  by  $H_{\text{eff}}$ , we can express those thermodynamical observables via the eigenvalues of the effective Hamiltonian

$$Z^{\text{eff}}(\beta) = \sum_{n=1}^N e^{-\beta E_n^{\text{eff}}},$$



Table 3. Comparison of the spectrum of the Klein-Gordon model on the lattice, between the MC Hamiltonian method with a *stochastic* basis and the analytic ones.

$n$	$E_n^{\text{eff}}$	$E_n^{\text{exact}}$
1	10.904663192168	10.944060480668
2	12.956830557334	12.944060480668
3	12.985023578737	13.057803869484
4	13.044311582647	13.057803869484
5	13.299967341242	13.321601993380
6	13.345480638394	13.321601993380
7	13.552195133687	13.589811791733
8	13.585794986361	13.589811791733
9	13.680136748933	13.751084748745
10	13.744919087477	13.751084748745
11	14.984737011385	14.944060480668
12	15.012353803145	15.057803869484
13	15.057295761044	15.057803869484
14	15.108904652020	15.171547258300
15	15.125356713561	15.171547258300
16	15.187413290039	15.171547258300
17	15.308536490102	15.321601993380
18	15.396255686587	15.321601993380
19	15.420708031412	15.435345382196
20	15.432823810789	15.435345382196

$$\begin{aligned}\overline{E}^{\text{eff}}(\beta) &= \sum_{n=1}^N \frac{E_n^{\text{eff}} e^{-\beta E_n^{\text{eff}}}}{Z^{\text{eff}}(\beta)}, \\ C^{\text{eff}}(\beta) &= k_B \beta^2 \left( \sum_{n=1}^N \frac{(E_n^{\text{eff}})^2 e^{-\beta E_n^{\text{eff}}}}{Z^{\text{eff}}(\beta)} - \left( \overline{E}^{\text{eff}}(\beta) \right)^2 \right).\end{aligned}\quad (22)$$

Since this is a static system, the eigenvalues should in principle not vary with  $\beta$ , which is also confirmed numerically within statistical errors when  $\beta$  and  $N$  are not too small. Using this assumption and the spectrum at  $\beta = 2$ , we obtain the thermodynamical quantities for other  $\beta$ . The results for the free energy, average energy and specific heat as a function of  $\beta$  are shown in Figs. 2, 3 and 4. Again, the results from the MC Hamiltonian are in good agreement with the analytical ones when  $\beta > 1$ .

Preliminary results for larger  $N_{\text{osc}}$  indicate that it is not necessary to

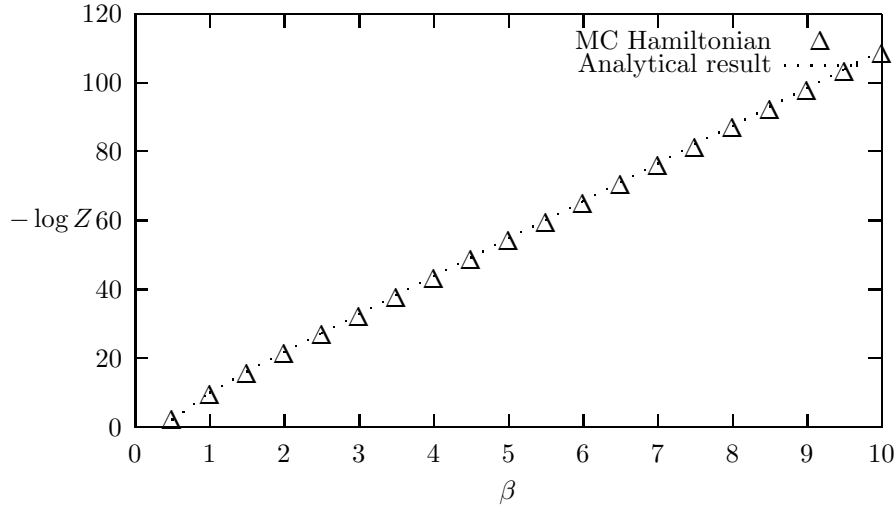


Figure 2. Free energy of the Klein-Gordon model on a 1+1 dimensional lattice.

increase  $N$  accordingly. This property is very important for a feasible application of the algorithm to many body systems and QFT.

## 5 Summary

In this paper, we have extended the effective Hamiltonian method with a stochastic basis to QFT, and taken the Klein-Gordon model as an example. The results are very encouraging. We believe that the application of the algorithm to more complicated systems will be very interesting for non-perturbative investigation beyond the ground state.

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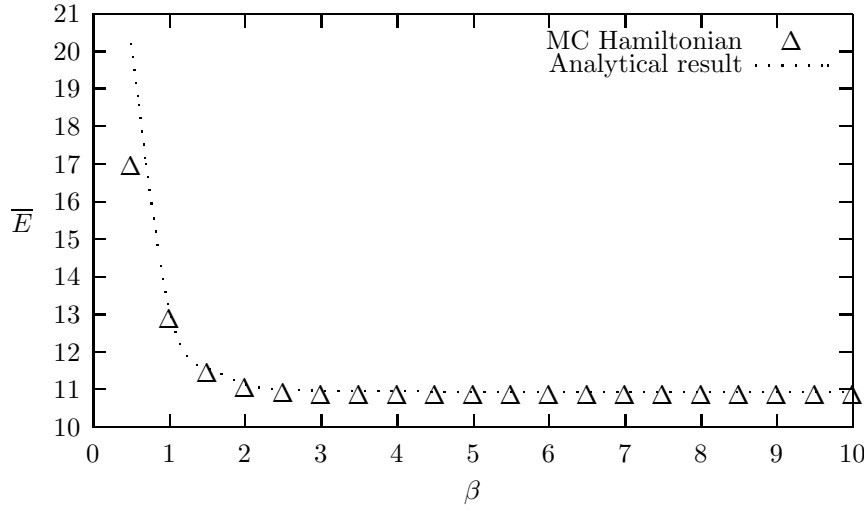


Figure 3. Average energy of the Klein-Gordon model on a 1+1 dimensional lattice.

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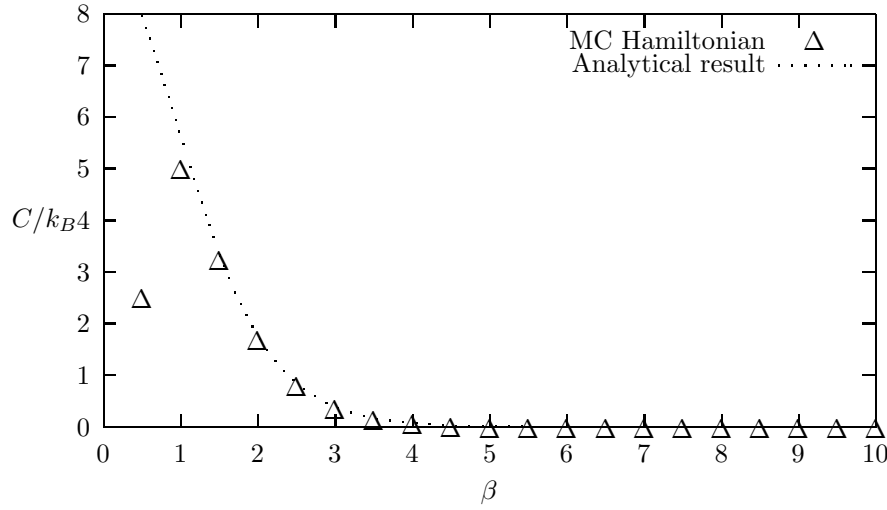


Figure 4. Specific heat over  $k_B$  of the Klein-Gordon model on a 1+1 dimensional lattice.

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